TRANSMITTAL FORM

(to be used for all correspondence after initial filing)

Application Number	10/053,348
Filing Date	November 2, 2001
First Named Inventor	Rosenthal, Dan E.
Art Unit	2123
Examiner Name	Unassigned

Total Number of Pages in This Submission	7	
Attorney Docket Number		020910-000310US

ENCLOSURES *(check all that apply)*

☐ Fee Transmittal Form	☐ Assignment Papers	☐ After Allowance Communication to Group
☐ Fee Attached	☐ Drawing(s)	☐ Appeal Communication to Board of Appeals and Interferences
☐ Amendment / Reply	☐ Licensing-related Papers	☐ Appeal Communication to Group **(Appeal Notice, Brief, Reply Brief)**
☐ After Final	☐ Petition Routing Slip (PTO/SB/69) and Accompanying Petition	☐ Proprietary Information
☐ Affidavits/declaration(s)	☐ Petition to Convert to a Provisional Application	☐ Status Letter
☐ Extension of Time Request	☐ Power of Attorney, Revocation Change of Correspondence Address	☒ Other Enclosure(s) (please identify below):
☐ Express Abandonment Request	☐ Terminal Disclaimer	Associate Power of Attorney
☒ Information Disclosure Statement	☐ Request for Refund	Return Receipt Postcard
☐ Certified Copy of Priority Document(s)	☐ CD, Number of CD(s) _____	45 references
☐ Response to Missing Parts/ Incomplete Application		
☐ Response to Missing Parts under 37 CFR 1.52 or 1.53		

Remarks	The Commissioner is authorized to charge any additional fees or credit any overpayment to Deposit Account 50-2599.

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SIGNATURE OF APPLICANT, ATTORNEY, OR AGENT

Firm or Individual	Protein Mechanics, Inc.	
	Charles K. Sholtz	Reg. No. 38,615
Signature	*[signature]*	
Date	March 21, 2003	

CERTIFICATE OF MAILING

I hereby certify that this correspondence is being facsimile transmitted to the USPTO or deposited with the United States Postal Service with sufficient postage as first class mail in an envelope addressed to: Commissioner for Patents, Washington, D.C. 20231 on this date: ___3/21/03___

Typed or printed	Charles K. Sholtz		
Signature	*[signature]*	Date	March 21, 2003

IN THE UNITED STATES PATENT AND TRADEMARK OFFICE

In re application of:	Examiner: Unassigned
Dan E. Rosenthal	Art Unit: 2123
Application No.: 10/053,348	SUPPLEMENTAL INFORMATION DISCLOSURE STATEMENT UNDER 37 CFR §1.97 and §1.98
Filed: November 2, 2001	
For: METHOD FOR ANALYTICAL JACOBIAN COMPUTATION IN MOLECULAR MODELING	

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Assistant Commissioner for Patents
Washington, D.C. 20231

Sir:

The references cited on attached form PTO/SB/08A and PTO/SB/08B are being called to the attention of the Examiner. Copies of the references are enclosed. It is respectfully requested that the cited references be expressly considered during the prosecution of this application, and the references be made of record therein and appear among the "references cited" on any patent to issue therefrom.

As provided for by 37 CFR 1.97(g) and (h), no representation is being made that a search has been conducted or that this statement encompasses all the possible relevant information, and no inference should be made that the information and references cited are, or are considered to be material to patentability because they are in this statement. No inference should be made that the information and references cited are prior art merely because they are in this statement.

Applicant believes that <u>no fee is required</u> for submission of this statement. However, if a fee is required, the Commissioner is authorized to deduct such fee from the undersigned's Deposit Account No. 50-2599. Please deduct any additional fees from, or credit any overpayment to, the above-noted Deposit Account.

Respectfully submitted,

Charles K. Sholtz
Reg. No. 38,615

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INFORMATION DISCLOSURE STATEMENT BY APPLICANT

(use as many sheets as necessary)

Complete if Known	
Application Number	10/053,348
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U.S. PATENT DOCUMENTS

Examiner	Cite No.[1]	Document Number — Number Kind Code[2] (if known)	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear
	AA	US 6,512,997	1/28/2003	Padilla, et al.	
	AB	US 6,185,506	2/6/2001	Cramer, III, et al.	
	AC	US 6,161,080	12/12/2000	Aouni-Ateshian, et al.	
	AD	US 6,125,235	9/26/2000	Padilla, et al.	
	AE	US 6,081,766	6/27/2000	Chapman, et al.	
	AF	US 6,014,449	1/11/2000	Jacobs, et al.	
	AG	US 5,787,279	7/28/1998	Rigoutsos	
	AH	US 5,777,889	7/7/1998	Mohanty, et al..	
	AI	US 5,752,019	5/12/1998	Rigoutsos, et al.	
	AJ	US 5,745,385	4/28/1998	Hinsberg, III, et al.	
	AK	US 5,625,575	4/29/1997	Goyal, et al.	
	AL	US 5,553,004	9/3/1996	Gronbech-Jensen, et al.	
	AM	US 5,307,287	4/26/1994	Cramer, III, et al.	

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FOREIGN PATENT DOCUMENTS

Examiner Initials*	Cite No.[1]	Foreign Patent Document — Country Code[3]	Number[4]	Kind Code[5] (if known)	Publication Date MM-DD-YYYY	Name of Patentee or Applicant of Cited Document	Pages, Columns, Lines, Where Relevant Passages or Relevant Figures Appear	T[6]
	AN	WO	02/073334	A2	07-26-1990	Padilla, et al.		☐
	AO	WO	01/67310	A1	12-12-1991	Smith, et al.		☐
	AP	WO	96/24902	A1	04-01-1993	Wertz		☐

OTHER PRIOR ART -- NON PATENT LITERATURE DOCUMENTS

Examiner Initials *	Cite No.[1]	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	T[2]
✓	AQ	ASCHER, et al., Computer Methods for Ordinary Differential Equations and Differential-Algebraic Equations, 1998, pgs. 3-122 and 231-297, SIAM, Philadelphia, PA.	
✓	AR	BARAFF, et al., "*Large steps in cloth simulation*", 1998, Computer Graphics Proceedings SIGGRAPH 98 (Orlando, July 19-24) p43.pdf	
	AS	BARTH, et al., "*A separating framework for increasing the timestep in molecular dynamics*" in Computer Simulation of Biomolecular Systems - Theoretical and Experimental Applications, Volume 3, 1997, pgs. 97-121, Kluwer AcademicDordrecht, The Netherlands.	

Examiner Signature		Date Considered	

*EXAMINER: Initial if reference considered, whether or not citation is in conformance with MPEP 609. Draw line through citation if not in conformance and not considered. Include copy of this form with next communication to applicant.

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√	AT	BERENDSEN, *"Molecular Dynamics Simulations: The Limits and Beyond"* in Computational Molecular Dynamics: Challenges, Methods, Ideas, 1999, pgs. 3-36, Springer-Verlang, Germany.	
√	AU	BISCHOF, et al., ADIFOR 2.0 Users' Guide, 1998, Argonne National Laboratory, University of Chicago, Argonne, IL.	
√	AV	BRENAN, et al., Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations, 1989, Chapter 5 (pgs. 115-148), Elsevier Science Publishing Co., New York, NY.	
√	AW	BUTCHER, *"Towards efficient implementation of singly-implicit methods"*, 1988, AMC Transactions of Mathematical Software 14:68-75.	
√	AX	BYSTROFF, *"An alternative derivation of the equations of motion in torsion space for a branched linear chain"*, 2001, Protein Engineering 14:825-828.	
√	AY	COLEMAN, et al., *"The efficient computation of sparse Jacobian matrices using automatic differentiation"*, 1996, Cornell Theory Center Technical Report CTC95TR225.	
	AZ	EICHBERGER, et al., *"The benefits of parallel multibody simulation"*, 1994, International Journal for Numerical Methods in Engineering, 37:1557-1572.	
√	BA	GOLUB, et al., *"The Differentiation of Pseudo-Inverses and Non-Linear Least Squares Problems Whose Variables Separate"*, 1973, SIAM J. Numer Anal. 10:413.	
√	BB	HAIRER, et al., Solving Ordinary Differential Equations II: Stiff and Differential-Algebraic Problems, 2nd ed., 1996, Springer-Verlang, Germany.	
√	BC	HE, et al., *"Macromolecular conformational dynamics in torsional angle space"*, 1998, Journal of Chemical Physics 108:271.	
√	BD	HOLLARS, et al., SD/FAST User's Manual, Version B.2, 1994, Symbolic Dynamics, California.	
√	BE	IZAGUIRRE, et al., *"Longer Time Steps for Molecular Dynamics"*, 1999, J.Chem.Phys. 110:9853.	
	BF √	KANE, Dynamics, 3rd ed., 1978, Stanford University, Stanford, California.	
	BG √	LEACH, Molecular Modelling Principles and Applications, 2nd ed., 1996, Chapter 6 (pgs. 303-352) Pearson Education Limited, England.	

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INFORMATION DISCLOSURE STATEMENT BY APPLICANT *(use as many sheets as necessary)*	Application Number	10/053,348
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Sheet 3 of 3	Attorney Docket Number	020910-000310US

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		OTHER PRIOR ART -- NON PATENT LITERATURE DOCUMENTS	
Examiner Initials *	Cite No.[1]	Include name of the author (in CAPITAL LETTERS), title of the article (when appropriate), title of the item (book, magazine, journal, serial, symposium, catalog, etc.), date, page(s), volume-issue number(s), publisher, city and/or country where published.	T[2]
✓	BH	MARTINS, et al., "*An automated method for sensitivity analysis using complex variables*", 2000, American Institute of Arenautics and Astronoautics, 2000-0689 p1	
✓	BI	NORSETT, et al., "*Embedded SDIRK-methods of basic order three*", 1984, BIT 24:634-646.	
✓	BJ	PONDER, TINKER User's Guide, Version 3.8, October 2000, Washington University, St. Louis, MO.	
✓	BK	RAPAPORT, The Art of Molecular Dynamics Simulation, 1995, reprinted with corrections 1998, Chapter 3 (pgs. 42-77), Cambridge University Press, United Kingdom.	
✓	BL	SCHLICK, "*Biomolecular Dynamics at Long Timesteps: Bridging the Timescale Gap Between Simulation and Experimentation*", 1997, Annu. Rev. Biophys. Biomol. Struct., 26:181-222.	
✓	BM	SCHLICK, "*Some Failures and Successes of Long-Timestep Approaches to Biomolecular Simulations*" in Computational Molecular Dynamics: Challenges, Methods, Ideas, 1999, pgs. 227-262, Springer-Verlang, Germany.	
	BN ✓	SCHLICK, Molecular Modeling and Simulation - An Interdisciplinary Guide, 2002, Chapter 13 and References, pgs. 419-462 and 561-619, Springer-Verlang, Germany.	
	BO ✓	SHAMPINE, "*Implementation of implicit formulas for the solution of ODEs*", 1980, SIAM J. Sci. Stat. Comput. 1:103-118.	
✓	BP	VERLET, "*Computer Experiments on Classical Fluids. I. Thermodynamical Properties of Lennard-Jones Molecules*", 1967, Physical Review, 159(1):98-103.	
✓	BQ	VON SCHWERIN, Multibody System Simulation, 1999, Springer-Verlang, Germany.	
✓	BR	WU, et al., "*Constraint dynamics algorithm for simulation of semiflexible macromolecules*", 1998, Journal of Computational Chemistry 19:1555-1566	
✓	BS	YEN, et al., "*On the numerical solution of constrained multibody dynamic systems*", 1994, University of Minnesota AHPCRC 94-038.	

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